JS 9/1/21
RJA 01/03/22

SAT Report for Case # P-18-0020

General

[redacted]

Report Status: Complete
Status Date: 01/28/2019
CRSS Date: 10/23/2017
SAT Date: 10/24/2017
SAT Chair: Legacy Placeholder
Consolidated PMN? N
Consolidated Set:
Submitter: Myriant Corporation
CAS Number: None
Ecotox Related Cases:
Health Related Cases: ANALOGS; [redacted]
Chemical Name: Butanedioic acid, polymer with 2-ethyl-2-(hydroxymethyl)-1,3-propanediol, 2,5-furandione and 1,3-propanediol, 3a,4,5,6,7,7a-hexahydro-4,7-methano-1H-inden-5(or 6)-yl ester
Use: [redacted] (by terminal groups).
Trade name: Myribond(R) DX
PV Max (kg/yr): 500000.0000
Ecotox Assessor: Gallagher, Jeffrey
Fate Assessor: Wong, Edmund
Health Assessor: Salazar, Keith

Physical Chemical Information

Molecular Weight:	535.00	**Physical State - Neat:**	Liquid		
Percent 500:	35.00	**Percent 1000:**	57.00		
Melting Point (Measured):		**Melting Point (est):**		**MPD (EPI):**	20.00
Vapor Pressure:		**Vapor Pressure (est):**	<0.000001	**VP (EPI):**	9.55e-010
Water Solubility:		**Water Solubility (EST):**	0.000019	**Water Solubility (EPI):**	
Log Kow:				**Log Kow (EPI):**	6.72
Log P:		**Log P Comment:**			

SAT Concern

Ecotox Rating (1):	1	**Ecotox Rating Comment (1):**	
Ecotox Rating (2):		**Ecotox Rating Comment (2):**	
Health Rating (1):	1	**Health Rating Comment (1):**	
Health Rating (2):		**Health Rating Comment (2):**	

PBT Ratings

Persistence	Bioaccumulation	Toxicity	Comments
3	1	1	

Exposure Based Review (Health)?	Y
Exposure Based Review (Ecotox)?	N
SAT Keywords:	None.

Fate Assessment Summary:	P-18-0020 FATE: Estimations for typical MW polymer, MW = 539, C31H38O8 Liquid with MP < 25 °C (E) log Kow = 6.72 (E) S = 0.019 mg/L at 25 °C (E) VP < 1.0E-6 torr at 25 °C (E) BP > 400 °C (E) H < 1.00E-8 (E) log Koc = 7.89 (E) log Fish BCF = 4.10 (13,000) (E) log Fish BAF = 1.15 (14) (E) POTW removal (%) = 90 via sorption Time for complete ultimate aerobic biodeg > mo Sorption to soils/sediments = v.strong PBT Potential: P3B1 *CEB FATE: Migration to ground water = negl Bioconcentration factor to be put into E-FAST: 14 PMN Material: Overall wastewater treatment removal is 90% via sorption. Sorption to sludge is strong based on the STP model output. Air Stripping (Volatilization to air) is negligible based on the estimated physical-chemical properties. Removal by biodegradation in wastewater treatment is negligible to

	moderate, with uncertainty. There was uncertainty due to the fact that the PMN is a polymer with a variable chemical structure. Depending on the structure and the terminated ends, the smaller pieces may biodegrade in wastewater treatment plants. The aerobic aquatic biodegradation half-life is greater than months based on structure. The anaerobic aquatic biodegradation half-life is greater than months based on the aerobic biodegradation half-life. The anaerobic biodegradation half-life is projected to be greater than or equal to the aerobic biodegradation half-life. Sorption to soil and sediment is very strong based on the estimated physical-chemical properties. Migration to groundwater is negligible based on the estimated physical-chemical properties. PMN Material: High Persistence (P3) is based on the estimated anaerobic biodegradation half-life. Low Bioaccumulation potential (B1) is based on the estimated Bioaccumulation factor (BAF). Bioconcentration/Bioaccumulation factor to be put into E-Fast: 14
Removal in WWT/POTW (Overall):	90

Condition	Rating Values w/ Rating Description	Comment
WWT/POTW Sorption:	3	
WWT/POTW Stripping:	4	
Biodegradation Removal:	4	
Biodegradation Destruction:		
Aerobic Biodeg Ult:	4	
Aerobic Biodeg Prim:		
Anaerobic Biodeg Ult:	4	

Condition	Rating Values w/ Rating Description	Comment
Anaerobic Biodeg Prim:		
Hydrolysis (t1/2 at pH 7,25C) A:		
Hydrolysis (t1/2 at pH 7,25C) B:		
Sorption to Soils/Sediments:	1	
Migration to Ground Water:	1	
Photolysis A, Direct:		
Photolysis B, Indirect:		
Atmospheric Ox A, OH:		
Atmospheric Ox B, O3:		

Health Assessment

Health Summary:	Absorption of the low molecular weight fraction (35% < 500, 57%< 1000) is poor all routes based on analogs.Although no significant health concerns were identified, there are no hazard data to confirm the expected low toxicity.
Routes of Exposure:	

Test Data Submitted

Test Data Submitted:	

Ecotox Assessment

Test organism	Test Type	Test Endpoint	Predicted	Measured	Comments
Fish	96-h	LC50	*		* = no effects at saturation. For the ecotoxicity endpoint value, predictions are based on ECOSAR (assessed structure had a molecular weight of 538; Parent PMN MW 535 with 35% <500 and 57% <1000)
Daphnid	48-h	LC50	*		* = no effects at saturation. For the ecotoxicity endpoint value, predictions are based on ECOSAR (assessed structure had a molecular weight of 538; Parent PMN MW 535 with 35% <500 and 57% <1000)
Green Algae	96-h	EC50	*		* = no effects at saturation. For the ecotoxicity endpoint value, predictions are based on ECOSAR (assessed structure had a molecular weight of 538; Parent PMN MW 535 with 35% <500 and 57% <1000)
Fish	-	Chronic Value	*		* = no effects at saturation. For the ecotoxicity endpoint value, predictions are based on ECOSAR (assessed structure had a molecular weight of

Test organism	Test Type	Test Endpoint	Predicted	Measured	Comments
					538; Parent PMN MW 535 with 35% <500 and 57% <1000)
Daphnid	-	Chronic Value	*		* = no effects at saturation. For the ecotoxicity endpoint value, predictions are based on ECOSAR (assessed structure had a molecular weight of 538; Parent PMN MW 535 with 35% <500 and 57% <1000)
Green Algae	-	Chronic Value	*		* = no effects at saturation. For the ecotoxicity endpoint value, predictions are based on ECOSAR (assessed structure had a molecular weight of 538; Parent PMN MW 535 with 35% <500 and 57% <1000)

Factors	Most Sensitive Endpoint	Assessment Factor	CoC	Comment
Acute Acquatic:				Because hazards are not expected up to the water solubility limit, acute and chronic concentrations of concern are not identified.
Chronic Acquatic:				Because hazards are not expected up to the water solubility limit, acute and chronic concentrations of concern are not identified.

No releases to water

Ecotox Route of Exposure?	

Factors	Values	Comments
SARs:	Esters	
SAR Class:	Esters-insoluble	
TSCA NCC Category?	Esters	

Recommended Testing

Ecotox
Value Comments

Predictions are based on QSARs for esters (ECOSAR V2.0; assessed structure had a molecular weight of 538; Parent PMN MW 535 with 35% <500 and 57% <1000); Log Kow = 6.72 (P, 538 MW); liquid with an unknown MP (P); S = 0.02 mg/L (P, 538 MW); effective concentrations based on 100% active ingredients and mean measured concentrations; hardness <150 mg/L as CaCO3; and TOC <2.0 mg/L.

Ecotox
Factors Comments

Environmental Hazard: Environmental hazard is relevant to whether a new chemical substance is likely to present unreasonable risks because the significance of the risk is dependent upon both the hazard (or toxicity) of the chemical substance and the extent of exposure to the substance. EPA estimated environmental hazard of this new chemical substance using the Ecological Structure Activity Relationships (ECOSAR) Predictive Model (https://www.epa.gov/tsca-screening-tools/ecological-structure-activity-releationships-ecosar-predictive-model); specifically the QSAR for esters (assessed structure had a molecular weight of 538; Parent PMN MW 535 with 35% <500 and 57% <1000). Acute and chronic toxicity values estimated for fish, aquatic invertebrates, and algae are all no effects at saturation. These toxicity values indicate that the new chemical substance is expected to have a low environmental hazard. Because hazards are not expected up to the water solubility limit, acute and chronic concentrations of concern are not identified.

Environmental Risk: Risks to the environment from acute and chronic exposure are not expected at any concentration of the new chemical substance soluble in the water (i.e., no effects at saturation).